chain nodes : 7 8 9 10 ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

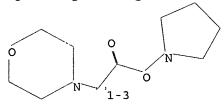
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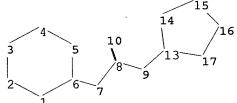
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 13:Atom 14:Atom 15:Atom 17:Atom

#### L1 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10765267pt2.str





chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

Match level :

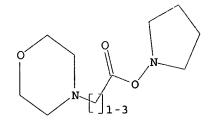
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 13:Atom 14:Atom 15:Atom 17:Atom

STRUCTURE UPLOADED L2

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 12

SAMPLE SEARCH INITIATED 15:00:11 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8 TO 329

PROJECTED ANSWERS: 0 TO

L3 0 SEA SSS SAM L2

=> d l1

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:00:34 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -8 TO ITERATE

100.0% PROCESSED 0 ANSWERS 8 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:00:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 172 TO ITERATE

100.0% PROCESSED 172 ITERATIONS 6 ANSWERS

SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
163.05
163.26

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FILE COVERS 1907 - 8 Sep 2005 VOL 143 ISS 11 FILE LAST UPDATED: 7 Sep 2005 (20050907/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6 4 L5

=> d ed abs ibib hitstr 1-4

ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 08 Oct 2004 ED

AB Provided is a method for characterizing a mol. by mass spectrometry, which mol. comprises one or more free amino groups, which method comprises: (a) reacting one or more free amino groups in the mol. with a mass tag reagent comprising a reactive functionality capable of reacting with an amino group, and a tertiary amino group linked to the reactive functionality; and (b) characterizing the mol. by mass spectrometry.

2004:824132 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

141:310231

TITLE:

Mass labels

INVENTOR(S):

Hamon, Christian; Kuhn, Karsten; Thompson, Andrew;

Reuschling, Dieter; Schaefer, Juergen

PATENT ASSIGNEE(S):

Xzillion G.m.b.H. & Co. K.-G., Germany; Proteome

Sciences PLC

SOURCE:

PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DAT	E A	PPLICATION NO.	DATE
WO 2004086050	A2 200	41007 W	O 2004-GB1167	20040318
WO 2004086050	A3 200	41229		
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GE, GH, GM	, HR, HU, ID	, IL, IN,	IS, JP, KE, KG,	KP, KR, KZ, LC,
LK, LR, LS	, LT, LU, LV	, MA, MD,	MG, MK, MN, MW,	MX, MZ, NA, NI,
NO, NZ, OM	, PG, PH, PL	, PT, RO,	RU, SC, SD, SE,	SG, SK, SL, SY,
TJ, TM, TN	, TR, TT, TZ	, UA, UG,	US, UZ, VC, VN,	YU, ZA, ZM, ZW
RW: BW, GH, GM	, KE, LS, MW	, MZ, SD,	SL, SZ, TZ, UG,	ZM, ZW, AM, AZ,
BY, KG, KZ	, MD, RU, TJ	, TM, AT,	BE, BG, CH, CY,	CZ, DE, DK, EE,
ES, FI, FR	, GB, GR, HU	, IE, IT,	LU, MC, NL, PL,	PT, RO, SE, SI,
SK, TR, BF	, BJ, CF, CG	, CI, CM,	GA, GN, GQ, GW,	ML, MR, NE, SN,
TD, TG				

PRIORITY APPLN. INFO.:

GB 2003-6756

A 20030324

741683-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(mass labels)

RN 741683-76-1 HCAPLUS

2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME)

$$\bigcap_{O} N - CH_2 - C - O - N$$

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Aug 2004

AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

ACCESSION NUMBER: 2004:681717 HCAPLUS

DOCUMENT NUMBER: 141:202794

TITLE: Methods, mixtures, kits and compositions pertaining to

analyte determination

INVENTOR(S): Pappin, Darryl J. C.; Bartlet-Jones, Michael

PATENT ASSIGNEE(S): Applera Corporation, USA SOURCE: PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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	WO	2004	0703	52		A2	_	2004	0819		WO 2	0 2004-US2077			20040127						
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			CU,	CU,	CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG,	ES,			
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			LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,	MW,	MX,	MX,			
			MZ,	MZ,	NA,	NI													•		
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			GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG									-		
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	US	2004	2196	85		<b>A1</b>		2004	1104		US 2	004-	7652	64		$\overline{}_2$	0040	127			
	US	2004	2204	12		A1		2004	1104		US 2	004-	7652	67—		2	0040	127			
	US	2004	2196	86		<b>A</b> 1		2004	1104		US 2	004-	7654	58		2	0040	127			
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Tm	7.4	1.000	76 3	n 74	1 - 0 -		~~ =														

IT 741683-76-1P 741683-77-2P 741683-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(methods, mixts., kits and compns. pertaining to analyte determination)

RN 741683-76-1 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME)

RN 741683-77-2 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)

RN 741683-78-3 HCAPLUS CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 30 May 1997 ED

AB The title polymers having a single reactive mojety at one end of the polymer chain have the following structure R-Z-X-Y (R = N-acryloylmorpholine residue with d.p. 6-280, which yields number-average mol. weight 1000-40,000; Z-X-Y = polymer capping moiety; X = saturated residue of linear or branched aliphatic series CrH2r, r = 1-12; Y = reactive moiety, such as -OH, -CO2H, or -NH2; Z = moiety that readily reacts to cap a polymer free radical, e.g., S). The monofunctional polymer is a suitable alternative to monofunctional PEG for modification of substances having biol. and biotech. applications.

1997:341994 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

127:34643

Polymers of N-acryloylmorpholine derivative activated TITLE: at one end and conjugates with bioactive materials and

surfaces

Veronese, Francesco M.; Schiavon, Oddone; Caliceti, INVENTOR(S):

Paolo; Sartore, Luciana; Ranucci, Elisabetta; Ferruti,

PATENT ASSIGNEE(S): Consiglio Nazionale Delle Ricerche, Italy

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				_	
US 5629384	Α	19970513	US 1994-243869		19940517
US 5631322	Α	19970520	US 1995-475177		19950607
PRIORITY APPLN. INFO.	:		US 1994-243869	<b>A3</b>	19940517

TT 190727-27-6P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); PRP (Properties); BIOL (Biological study); PREP (Preparation)

(polymers of N-acryloylmorpholine derivative activated at one end and conjugates with bioactive materials and surfaces)

RN190727-27-6 HCAPLUS

Morpholine, 4-[4-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1,4-dioxo-2-butenyl]-, CN homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 190727-26-5 CMF C12 H14 N2 O6

L6 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 12 May 1984

GI

AB Spectinomycylamines I [R = alkyl, optionally substituted CH2Ph, cyclohexyl, oxoalkyl, hydroxyalkyl, optionally substituted benzoylalkyl, acyl, aminoalkyl, amino(hydroxy)alkyl, amino(oxo)alkyl, carbamoylphenyl; R1 = H, Me] were prepared and showed bactericidal activity. Thus 6,8-bis(benzyloxycarbonyl)spectinomycin was treated with Me2CHNH2 and NaB(CN)H3, and the product was subjected to hydrogenolysis to give I (R = CHMe2, R1 = H), which had a ED50 against Escherichia coli ATCC 11775 of 9 mg/kg s.c. in mice.

ACCESSION NUMBER: 1980:639849 HCAPLUS

DOCUMENT NUMBER: 93:239849

TITLE: Spectinomycylamines and pharmaceutical compositions

containing them

INVENTOR(S): Woitun, Eberhard; Maier, Roland; Reuter, Wolfgang;

Wetzel, Bernd; Goeth, Hanns; Lechner, Uwe; Werner, Uwe

PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 102 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: Facence

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2851953	A1	19800619	DE 1978-2851953		19781201
PRIORITY APPLN. INFO.:			DE 1978-2851953	Α	19781201
IT 75727-76-3					

RL: RCT (Reactant); RACT (Reactant or reagent)

(N-acylation of bis(benzyloxycarbonyl)spectinomycylamine by)

RN 75727-76-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[3-(4-morpholinyl)-1-oxopropoxy]- (9CI) (CA INDEX NAME)

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	24.66	187.92
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	ENTRY	SESSION
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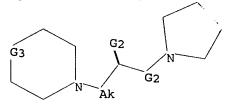
STN INTERNATIONAL LOGOFF AT 15:01:51 ON 08 SEP 2005

=> screen 2039

### L1 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\expand10765267.str



chain nodes :
7 8 9 10
ring nodes :

1 2 3 4 5 6 11 12 13 14 15

chain bonds :

6-7 7-8 8-9 8-10 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 6-7 \quad 7-8 \quad 8-9 \quad 8-10 \quad 9-11 \quad 11-12 \quad 11-15 \quad 12-13 \quad 13-14$ 

14-15

isolated ring systems :

containing 1 : 11 :

G1:C,N

G2:0,S

G3:C,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom

L2 STRUCTURE UPLOADED

=> que L2 AND L1

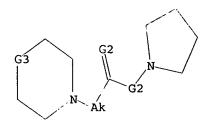
L3 QUE L2 AND L1

=> d 13

L3 HAS NO ANSWERS

L1 SCR 2039

L2 STR



G1 C,N G2 O,S

·G3 C,O,N

Structure attributes must be viewed using STN Express query preparation. L3  $\,$  QUE  $\,$  L2 AND  $\,$  L1

=> s 13

SAMPLE SEARCH INITIATED 15:50:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L2 AND L1

=> s 13 full

FULL SEARCH INITIATED 15:50:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 9 ANSWERS

SEARCH TIME: 00.00.01

L5 9 SEA SSS FUL L2 AND L1

=> fil hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 164.77 164.98

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FILE COVERS 1907 - 8 Sep 2005 VOL 143 ISS 11 FILE LAST UPDATED: 7 Sep 2005 (20050907/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15 L6 7 L5

=> d ed abs ibib hitstr 1-7

ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 08 Jul 2005 ED

GI

EFO 1/30/03

AΒ Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, anamino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

ACCESSION NUMBER:

2005:592130 HCAPLUS

DOCUMENT NUMBER:

143:115574

TITLE:

Preparation of isotopically enriched N-substituted

piperazines

INVENTOR (S):

Pappin, Darryl J. C.; Pillai, Sasi; Coull, James M. Applera Corp., USA
U.S. Pat. Appl. Publ. 29 pp.
CODEN: USXXCO
Patent

PATENT ASSIGNEE(S):

SOURCE:

LANGUAGE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT:

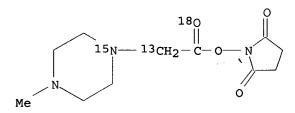
PATENT INFORMATION:

PATENT NO.

KIND DATE APPLICATION NO.

DATE

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20050707
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     US 2005148773
                           A1
                                                                       20040105
     WO 2005068446
                           A1
                                 20050728
                                              WO 2005-US223
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             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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PRIORITY APPLN. INFO.:
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                                              US 2004-852730
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                                                                       20040524
IT
     856188-20-0P
     RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
     (Analytical study); PREP (Preparation); USES (Uses)
        (preparation of isotopically enriched N-substituted piperazines as isobaric
        labeling reagents)
     856188-20-0 HCAPLUS
RN
     2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-
CN
     180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)
```



#### •2 HCl

#### 

•2 HCl

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 08 Jul 2005 ED

GI

In some embodiments, this invention pertains to active esters of AB N-substituted piperazine acetic acid I (R = leaving group; X = 0, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 180H) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

ACCESSION NUMBER:

2005:592129 HCAPLUS

DOCUMENT NUMBER:

143:97398

TITLE:

Preparation of active esters of N-substituted piperazine acetic acids, including isotopically

enriched versions

INVENTOR(S):

Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha,

Subhasish; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S):

Applera Corp., USA

U.S. Pat. Appl. Publ., 33 pp.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

SOURCE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		APPLICATION NO.	DATE			
US 2005148771	A1 200507	07 US 2004-751354	20040105			
WO 2005068446	A1 200507:	28 WO 2005-US223	20050105			
W: AE, AG, AL,	AM, AT, AU, A	Z, BA, BB, BG, BR, BW,	BY, BZ, CA, CH,			
CN, CO, CR,	CU, CZ, DE, D	K, DM, DZ, EC, EE, EG,	ES, FI, GB, GD,			
GE, GH, GM,	HR, HU, ID, I	L, IN, IS, JP, KE, KG,	KP, KR, KZ, LC,			
LK, LR, LS,	LT, LU, LV, M	A, MD, MG, MK, MN, MW,	MX, MZ, NA, NI,			
NO, NZ, OM,	PG, PH, PL, P	r, RO, RU, SC, SD, SE,	SG, SK, SL, SY,			
TJ, TM, TN,	TR, TT, TZ, U	A, UG, US, UZ, VC, VN,	YU, ZA, ZM, ZW			
RW: BW, GH, GM,	KE, LS, MW, M	Z, NA, SD, SL, SZ, TZ,	UG, ZM, ZW, AM,			
AZ, BY, KG,	KZ, MD, RU, To	J, TM, AT, BE, BG, CH,	CY, CZ, DE, DK,			
EE, ES, FI,	FR, GB, GR, H	J, IE, IS, IT, LT, LU,	MC, NL, PL, PT,			
RO, SE, SI,	SK, TR, BF, B	J, CF, CG, CI, CM, GA,	GN, GQ, GW, ML,			
MR, NE, SN,	TD, TG					
PRIORITY APPLN. INFO.:		US 2004-751353	A 20040105			
		US 2004-751354	A 20040105			
		US 2004-751387	A 20040105			
		US 2004-751388	A 20040105			
		US 2004-822639	A 20040412			
		US 2004-852730	A 20040524			

IT 856187-87-6P 856188-16-4P 856188-20-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ N & & \\ N & & \\ \end{array}$$

RN 856188-16-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

## ●2 HCl

RN 856188-20-0 HCAPLUS

CN

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

#### ●2 HCl

ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6 ED Entered STN: 08 Jul 2005 This invention pertains to mixts. of isobarically labeled analytes and AR fragment ions thereof. ACCESSION NUMBER: 2005:592027 HCAPLUS DOCUMENT NUMBER: 143:93642 Mixtures of isobarically labeled analytes and TITLE: fragments ions derived therefrom Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, INVENTOR(S): James M. PATENT ASSIGNEE(S): Applera Corp., USA U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. SOURCE: Ser. No. 751,353. CODEN: USXXCO DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE ---------\_\_\_\_\_\_ **A1** 20050707 US 2004-822639 US 2005147985 20040412 US 2004-751353 US 2005147982 A1 20050707 20040105 US 2004-852730 US 2005148087 20050707 20040524 A1 WO 2005068446 A1 20050728 WO 2005-US223 20050105 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG PRIORITY APPLN. INFO.: US 2004-751353 A2 20040105 US 2004-751354 A 20040105 US 2004-751387 A 20040105 US 2004-751388 A 20040105 US 2004-822639 A2 20040412 US 2004-852730 A 20040524 856187-87-6P 856188-16-4P 856188-20-0P IT RL: SPN (Synthetic preparation); PREP (Preparation) (mixts. of isobarically labeled analytes and fragments ions derived therefrom) RN856187-87-6 HCAPLUS 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) CN(CA INDEX NAME)

RN 856188-16-4 HCAPLUS CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-,

dihydrochloride (9CI) (CA INDEX NAME)

## •2 HCl

RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

L6 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

GI

AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y =straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

ACCESSION NUMBER: 2005:588426 HCAPLUS

DOCUMENT NUMBER: 143:115568

TITLE: Preparation of isotopically enriched N-substituted

piperazine-1-acetic acids

INVENTOR(S): Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha,

Subhasish; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S): Applera Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PA	PATENT NO.														DATE					
	2005									***************************************					20040705					
				A1 20050707			US 2004-751387													
WO	2005	0684	46		A1		2005	0728	WO 2005-US223						20050105					
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,			
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		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,			
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,			
		TJ,	TM,	TN,	TR,	TT,	ΤZ,	UA,	ŪĠ,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
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		MR,	ΝE,	SN,	TD,	TG														
PRIORIT	Y APP	LN.	INFO	.:					1	US 2	004-	7513	53		A 2	0040	105			
									1	US 2	004-	7513	54		A 2	0040	105			
									1	US 2	004-	7513	87		A 2	0040	105			
							US 2004-751388							A 2	0040	105				
								US 2004-822639					4	A 2	4 20040412					
									US 2004-852730						A 20040524					
			_																	

#### IT 856188-20-0P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

#### ●2 HCl

#### IT 856188-16-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856188-16-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

## ●2 HCl

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to isobarically labeled analytes and fragment ions

thereof.

ACCESSION NUMBER: 2005:588349 HCAPLUS

DOCUMENT NUMBER: 143:112150

TITLE: Isobarically labeled analytes and fragment ions

derived therefrom

INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull,

 ${\tt James}\ {\tt M}.$ 

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S.

Ser. No. 822,639.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT	NO.	KIND	DATE	APPLICATION NO.	DATE			
110 2005	148087	7.1	20050707	US 2004-852730	20040524			
	:							
US 2005	147982	A1	20050707	US 2004-751353	20040105			
US 2005	147985	A1	20050707	US 2004-822639	20040412			
WO 2005	068446	A1	20050728	WO 2005-US223	20050105			
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	GE, GH, GM,	HR, HU,	ID, IL,	IN, IS, JP, KE, KG,	KP, KR, KZ, LC,			
	LK, LR, LS,	LT, LU,	LV, MA,	MD, MG, MK, MN, MW,	MX, MZ, NA, NI,			
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	TJ, TM, TN,	TR, TT,	TZ, UA,	UG, US, UZ, VC, VN,	YU, ZA, ZM, ZW			
RW:	BW, GH, GM,	KE, LS,	MW, MZ,	NA, SD, SL, SZ, TZ,	UG, ZM, ZW, AM,			
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	EE, ES, FI,	FR, GB,	GR, HU,	IE, IS, IT, LT, LU,	MC, NL, PL, PT,			
	RO, SE, SI,	SK, TR,	BF, BJ,	CF, CG, CI, CM, GA,	GN, GQ, GW, ML,			
	MR, NE, SN,	TD, TG						
PRIORITY APP	LN. INFO.:			US 2004-751353	A2 20040105			
				US 2004-822639	A2 20040412			
				US 2004-751354	A 20040105			
				US 2004-751387	A 20040105			
				US 2004-751388	A 20040105			
				US 2004-852730	A 20040524			

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(isobarically labeled analytes and fragment ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 08 Jul 2005 ED

This invention pertains to mixts. of isobarically labeled analytes and AB fragment ions thereof.

ACCESSION NUMBER: 2005:588336 HCAPLUS

DOCUMENT NUMBER:

143:93635

TITLE:

SOURCE:

Mixtures of isobarically labeled analytes and

fragments ions derived therefrom

Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, INVENTOR(S):

James M.

PATENT ASSIGNEE(S):

Applera Corporation, USA U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	PATENT NO. KIND DATE				APPLICATION NO.						DATE							
us	2005	14798	32		A1	-	2005	0707		US 2	2004-	7513	53		20	0040	105	
US	2005	14798	35		A1		2005	0707	US 2004-822639						20040412			
US	2005	1480	37		A1	20050707			US 2004-852730						20040524			
WO	2005	06844	16		A1		2005	0728		WO 2	2005-1	JS22:	3		20	0050	105	
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PRIORITY	APP	LN.	INFO	. :						US 2	2004-	7513	53	I	A2 2	0040	105	
										US 2	2004-'	7513	54	Ĩ	A 20	0040	105	
										US 2	2004-	7513	87	Ž	A 2	0040	105	
										US 2	2004 -	7513	88	i	A 2	0040	105	
										US 2	2004-	8226	39	i	A2 2	0040	412	
										US 2	2004-	8527	30	i	A 2	0040	524	

IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-87-6 HCAPLUS

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) CN (CA INDEX NAME)

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ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
L6
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Entered STN: 20 Aug 2004 ED

AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

ACCESSION NUMBER: 2004:681717 HCAPLUS

DOCUMENT NUMBER: 141:202794

TITLE: Methods, mixtures, kits and compositions pertaining to

analyte determination

INVENTOR (S): Pappin, Darryl J. C.; Bartlet-Jones, Michael

PATENT ASSIGNEE(S): Applera Corporation, USA SOURCE: PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION: DAMENTO MA

P	PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
						-									_			
W	0 2004	0703	52		A2		2004	0819	1	WO 2	004-1	JS20	77		2	0040	127	
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		LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,	MW,	MX,	MX,	
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C	A 2488	584			AA		2004	0819	1	CA 2	004-2	2488	584		2	0040	127	
U:	S 2004	2196	85		A1		2004	1104	1	US 2	004-	7652	64		2	0040	127	
U:	S 2004	2204	12		A1		2004	1104	1	US 2	004-	7652	67/	<b>7</b>	2	0040	127	
U:	S 2004	2196	86		A1		2004	1104	1	US 2	004-	7654	58	1	2	0040	127	
PRIORI'	TY APP	LN.	INFO	. :					1	US 2	003-4	4436	12P	/	P 2	0030	130	
									1	WO 2	004-1	JS20	77	/ 1	W 2	0040	127	

IT 741683-77-2P 741683-78-3P 741683-86-3P 741683-93-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(methods, mixts., kits and compns. pertaining to analyte determination)

RN 741683-77-2 HCAPLUS

2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX CNNAME)

RN 741683-78-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)

RN 741683-86-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)

RN 741683-93-2 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)

=> log y		
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	ENTRY	SESSION
FULL ESTIMATED COST	37.03	202.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.11	-5.11

STN INTERNATIONAL LOGOFF AT 15:51:21 ON 08 SEP 2005